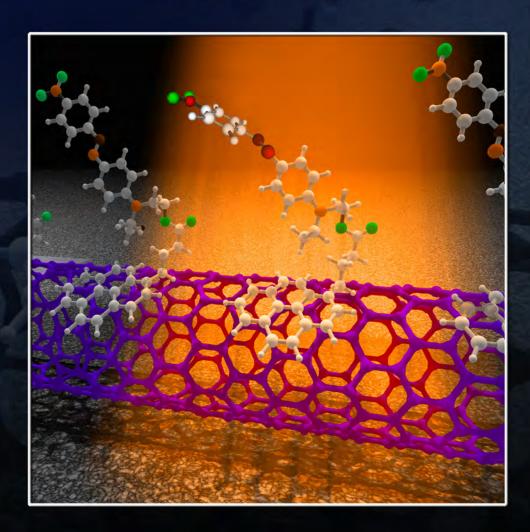


Laboratory Directed Research and Development

# 2010 Highlights







projects that were ongoing in 2010. Featured are research highlights of the recipients of LDRD Awards for Excellence. These are awards given to a small number of our Pls to acknowledge some of the outstanding work in the program and the impact it is having on mission execution.

# CTO and Vice President Science, Technology, and Engineering Research Foundations jsrottl@sandia.gov 505-844-3882

#### **About LDRD**

Maintaining Sandia's world-class science, technology, and engineering capabilities and anticipating their evolution in response to future challenges are absolutely essential to the Laboratories' ability to address national security needs. Authorized by Congress in 1992, the Laboratory Directed Research and Development (LDRD) Program reflects precisely that congressional intent — to encourage and sustain preeminent science and technology by investing in high-risk, potentially high-payoff research and development. The program is designed to proactively anticipate the breadth and depth of research and technological development that oncoming challenges will require

LDRD projects seek innovative technical solutions to our nation's most-significant challenges, often in collaboration with corporate and academic partners. LDRD allows Sandia to recruit and retain outstanding scientific and engineering talent in service to the Laboratories' five primary strategic business areas: nuclear weapons; energy resources and nonproliferation; defense systems and assessments; homeland security and defense; and science, technology, and engineering foundations.

For further information, contact:
Henry R. Westrich

LDRD Program Manager
hrwestr@sandia.gov

505-844-9092

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#### **Cover Image:**

Drawing of single wall carbon nanotube showing dye molecules noncovalently bound to the nanotube wall; the cis-trans isomerization of the dye upon light absorption accounts for changes in voltage and current flow in this nanostructure (for story, see page 5 of this publication). Here, the approximate conformational diffrence in the isomers is illustrated, with the cis isomer at center and the trans isomer at left.

# 2010 LDRD Award for Excellence Winners:

5, 6, 9, 13, 14, 20, 24

Writer Vin LoPresti Sandia Staffing Alliance, LLC

Graphic Design Chris Brigman Sandia National Laboratories



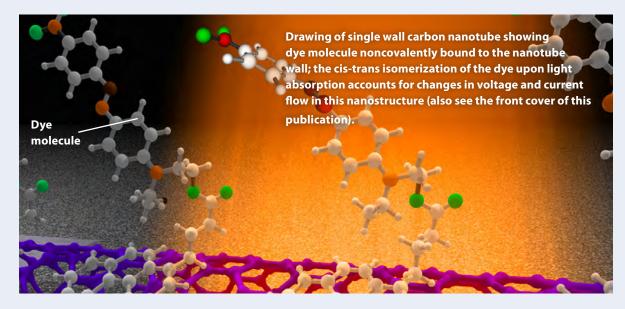


# Energy Conversion using Chromophore-functionalized Carbon Nanotubes Andrew Vance

he transformation of light (electromagnetic) energy into electrical or ionic currents is a key step in several biological processes (vision, photosynthesis) as well as the critical step in photovoltaic technologies. Within this field of optoelectronics, single wall carbon nanotubes (SWCTs) offer several attractive features because of their direct bandgaps and also the possibility of ballistic electron transport (electron motion with negligible scattering effects). Unfortunately, photoelectric transformation in carbon nanotubes has generally been limited to irradiation at high intensity, such as in the case of laser illumination of the nanotubes, whose range of spectral response is limited. This project sought to chemically modify carbon nanotubes in order to render them sensitive to lower light intensity, as well as to seek to target the response to specific regions of the optical spectrum, and to characterize this behavior at a fundamental level.

Prior LDRD-funded research in this area had indicated that a chromophore-functionalized nanotube could function as a light-switched electrical current conductor,

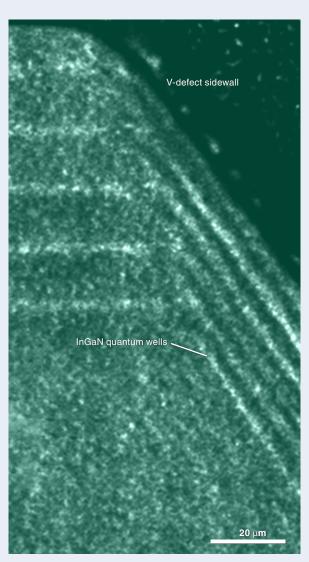
and this project leveraged that result by illustrating that nanoscale color photodetection at low intensities was possible. This was achieved by noncovalently modifying nanotubes with different chromophores, chemical variants of azobenzene. By choosing different chromophores, the project investigators obtained optical detection (a voltage difference across the nanotube) in specifically targeted regions of the visible spectrum. Evaluating the source of this voltage indicated that the optical switching resulted from the cis-trans isomerization of the chromophores, with a relatively small change in the electrostatic potential between the two isomers amplified into a larger voltage shift. This result verified that chromophore-modified SWCTs can transduce the photoabsorption-induced chromophore isomerization into electrical signals at low light intensity, and with color (wavelength) selectivity within the visible spectrum. Ongoing work has utilized these findings to fabricate chromophorenanotube p-n junction photovoltaic devices, utilizing modeling to enable discovery of chromophores in the upper visible and nearinfrared spectral regions. ■



# Nanoengineering for Solid State Lighting (and Other Applications) Mary Crawford

n an era of diminishing energy resources and global climate change, solid-state lighting is a key technology. If LED electricalto-optical energy conversion efficiency goals of 50% or greater could be achieved, worldwide electricity consumption due to lighting could be decreased by more than 50%, total consumption of electricity by more than 10%. Yet, a fundamental challenge involves understanding the nanoscale science that governs light generation and extraction from visible LED semiconductor materials and developing nanoscale engineering concepts to achieve the significant increases in LED optical efficiency that are required to make global SSL a commercial reality. In addition, UV semiconductor lasers have key applications in biological/chemical threat detection. The research outcomes produced in this project have brought a breadth and depth of clarity to the solid state lighting community, publicized through not only scholarly publications but also through partnership with Rensselaer Polytechnic Institute (RPI) and through the National Institute for Nano Engineering (NINE).

This team undertook a group of fundamental studies aimed at improving the efficiency of light emission from indium gallium nitride (InGaN) light-emitting pn-junctions, critical to LEDs and semiconductor injection lasers. One set of investigations aimed at understanding factors limiting internal quantum efficiency (IQE), with an emphasis on nanoscale defects, and other research initiatives experimented with nanoengineering approaches to increasing light extraction. A major emphasis was the study of LED efficiency droop at high currents, concluding the absence of a strong dependence on threading dislocation density, and consistent with a carrier leakage explanation. Other investigations shed new light on the controversy surrounding the relationship between v-defect



Micrograph of quantum wells at the edge of a V-defect in indium gallium nitride

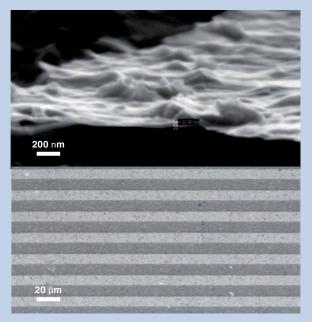
density and IQE. A further study explained the anomalous ideality factors of InGaN LEDs as relating to internal polarization fields. In parallel, several advanced light extraction methods employed nanoscale engineering of dielectric or metallic materials, especially light-extraction efficiency enhancement via graded-refractive-index coatings. Significant enhancement of light emission from InGaN quantum wells via coupling to surface plasmons in a nanopatterned metal coating was also demonstrated.

#### **Responsive Nanocomposites**

#### **Tim Boyle**

The design of materials that respond to changing environmental conditions with altered physical and/or chemical properties is a leading-edge materials area that will impact fundamental scientific as well as several Sandia mission areas, particularly where nanocomposites are utilized, including energy security and weapons. For example, polymeric materials in gasket seals would adapt to differing temperatures and humidity such that they maintain an optimal degree of functionality regardless of climate variations.

As a fundamental incursion into this nascent field, this project includes collaborations with numerous academic partners, allowing diverse experimental and modeling exploration of various nanoparticle-polymer composites, including, for example, metals and electrospun polyvinylpyrrolidone, graphene-titania — whose self-assembling films are photoresponsive — and alkylsilane-coated silica nanoparticles with organic molecules such as squalene (model elastomer). Industrial collaborators, such as Goodyear™, Exxon/Mobil™, and Intel™ are potential customers for project outcomes.



Electron micrographs of a graphene- ${\rm TiO_2}$  composite (top) that self-assembles at a liquid-air interface and shows photoresponsive characteristics when deposited on an interdigitated electrode (bottom).

#### Interfacial Electron and Phonon Scattering Processes in High-powered Nanoscale Applications

#### **Patrick Hopkins**

Large heat fluxes generated during the operation of nanoelectronics systems have become a significant limiting factor because inadequate heat dissipation increases operating temperature, thus degrading performance and shortening device lifetime. With ongoing decreases in size of such systems, thermal management issues increasingly arise at interfaces between different materials, where energy carrier scattering is prominent. This problem is even more pronounced in high-powered systems such as modern weapons, sensors, signal processors, and energy-conversion systems.

This project has examined these phenomena at a fundamentalphysics level, both through modeling and experiment, using the techniques of time-domain thermoreflectance (TDTR)

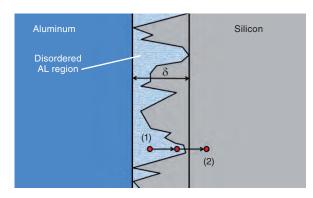


Diagram of dynamics at a silicon-aluminum interface with a disordered interfacial region of aluminum, treated as a crystalline region with grain size,  $\delta$ .

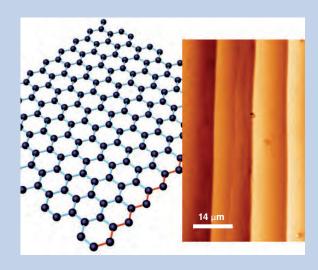
and measurements of interfacial phonon scattering. Results indicate that in electric-field-directed convective assembly of titanium dioxide nanoparticle films, thermal conductivity is very low, is tunable, and can be explained by phonon scattering at nanoparticle boundaries. Given that phononic crystals can control phonon dispersion, utilizing such crystals to control thermal transport in nanosystems provides a means of reducing thermal conductivity.

### **Enabling Graphene Nanoelectronics**

#### **Stephen Howell**

A single layer of hexagonally bonded carbon atoms, graphene's high-performance electronic properties, its physical strength, potential for band gap manipulation and other properties make it a promising candidate as a novel semiconductor in nanoelectronics. However, techniques must be developed to reproducibly deposit and/or synthesize high-quality graphene onto wafer-scale areas. Given the paucity of fundamental knowledge about graphene formation and defects that may arise, the genesis of such large-area graphene sheets is a daunting proposition.

This project is pursuing multiple approaches to synthesize reduced-defect graphene sheets and transferring them to other surfaces, the goal to produce graphene with ever-higher carrier mobility, predicted to be as high as ~200,000 cm²/Vsec because of quantum electrodynamic effects. The project has formed graphene by thermal decomposition of silicon carbide, and nucleated the vapor on different metals. In addition, the team



Graphene molecular structure (left) and micrograph of layered graphene sheets grown on silicon carbide (right).

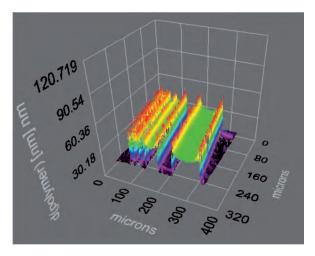
has been successful in transferring graphene to glass substrates and characterizing properties using low energy electron microscopy (LEEM), Raman spectroscopy, and measurements of electronic transport, during which the integer quantum Hall effect has been observed.

#### Nanolithography by Combined Self-Assembly and Directed-Assembly

#### **Dale Huber**

Creating defined nanoscale patterns is fundamental to the microelectronics industry—microchips and information storage devices—as well as exhibiting potential applications in other areas such as nanofluidics. Standard approaches to patterning involve lithography, with shorter wavelengths of irradiation utilized for nanopatterning, techniques that are expensive, time-consuming, and limited in the scope of potential patternable materials.

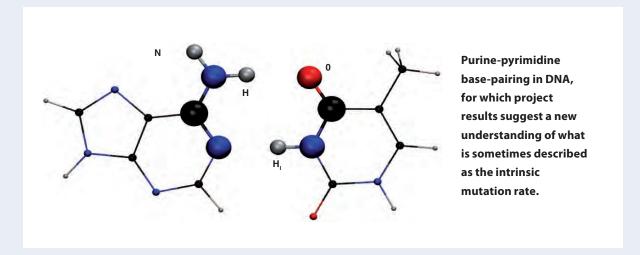
This project is developing an inexpensive approach toward creating directionally aligned nanoscale patterns on a variety of surfaces, utilizing micron-scale directed assembly to drive nanoscale self-assembly. Micron-sized features are lithographically defined (by soft lithography or standard UV lithography, and a mixed polymer monolayer is synthesized within these defined features. Nanoscale phase separation of the mixed polymer layer within the feature can yield a variety of



Measurements of extent of polymer growth from a surface nanopatterned by phase separation of a mixed polymer growth initiator.

nanopatterned surfaces as initiators upon which to grow further polymers, depending upon the specific parameters of phase separation, with features tens of nanometers in scale.

# Computational Schemes for Predictive Modeling and Engineering of Materials Anatole Von Lilienfeld



he ability to accurately model atomic and molecular systems is key to predicting and designing materials for particular applications without conducting laborious experimental protocols. For example, the Sandia solar-thermal tower employs a molten salt to store thermal energy from sunlight, later releasing it to drive a mechanical engine that turns an electrical generator, thus converting sunlight to electricity. The salt can be heated to 600 °C, but at the top of the tower, temperatures at or above 1000 °C are reached; problematically the salt decomposes, losing its chemical structure above 600 °C. Additionally, the salt remains liquid — able to flow through the system's pipes — only above 100 °C, and it must be heated to the boiling point of water at night. What if a salt could be found that remained liquid at room temperature and absorbed the maximum amount of available solar thermal energy without decomposing? A daunting task to an experimentalist, it becomes more tractable with computational modeling, predicting desired properties directly from structural, bonding and quantum considerations.

Bridging statistical mechanics, density functional theory (DFT), and

computer science, this young and highly interdisciplinary field of atomistic computational materials design has, in this project, been used to investigate several important Sandia energy-security areas. In addition to the heat-transfer fluids just described, nanocluster metal catalysts were studied for efficient conversion of carbon dioxide, methane, or oxygen for sustainable energy applications, and quantitative structureproperty relationships were developed for rapid but accurate predictions of charge transport properties in photovoltaic applications. At a more-fundamental level, high-dimensional property gradients in compound space were derived within density functional theory (DFT), and implemented and tested numerically. Interatomic three-body van der Waals forces, typically neglected, were shown to be substantial in real materials. Also examined were intrinsic defects in GaAs, and long range interactions in nanoscale sciences. This research furthered the accuracy of computational materials modeling, a key step forward toward routinely engineering improved materials prior to attempting experimental realization.

Computation and Simulation

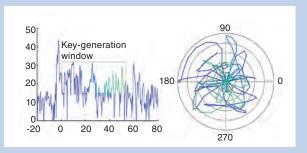
# SANDIA NATIONAL LABORATORIES

#### The Generation of Cryptographic Keys through Impulse Response Estimation

#### **Michael Forman**

Private-key cryptography—algorithms by which data is encrypted before transmission, then decrypted at its destination—employs a class of algorithms that use an identical key for both encryption and decryption. Because this key must be private and at the same time, distributed among communicating nodes, a secure key-distribution infrastructure is required. Such an infrastructure is infeasible in certain scenarios, and in these cases, alternative methods for managing keying variables have been proposed, one of which utilizes the communications channel itself to generate a keying variable; this eliminates eavesdropping, because third-parties do not share that same communication channel.

This project developed a system for generating data for cryptography from the characteristics of the transmission channel, data that remains private to transmitter and receiver of



A measurement of channel activity from which numerous vectors extracted from a key-generation window provide adequate binary data for use as private cryptography keys.

the encrypted information. The research has established a test bed for cryptography that could enable secure communications in ad hoc scenarios — such as a battlefield or in the deployment of scattered sensors) where a key-management system is otherwise unavailable.

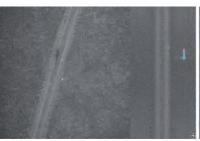
#### **Velocity Independent Continuous Tracking Radar**

#### **David Harmony**

Airborne ground-imaging radars suffer from a "velocity blindness." Because of the different processing intervals utilized for ground moving target indication (GMTI) as compared with stationary synthetic aperture radar (SAR), there are velocity regions where vehicles cannot be imaged and detected. Obviously, these blind spots create problematic security gaps. For example, following individual vehicles over typical velocity changes experienced while maneuvering in traffic is extremely

difficult. When a vehicle slows or stops, tracking becomes virtually impossible for present systems.

This project's goal was to develop algorithms creating an integrated model that combines videoSAR and GMTI signal processing from a single data stream to eliminate such velocity gaps and then implement the algorithms into real-time radar software to evaluate their performance. The desired outcome is a new radar mode similar to optical full motion video, but with the capability of night and day all-weather vehicle tracking independent of target velocity.







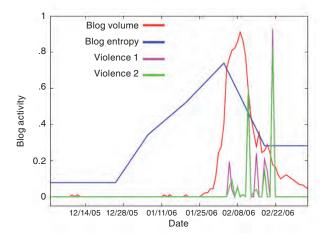
Three frames tracking vehicle movement along a road (left of each frame). Vehicle (arrow) is stopped, but nonetheless imaged in the middle frame.

#### Network Discovery, Characterization, and Prediction

#### Philip Kegelmeyer

"Our adversaries are networks," is a key theme articulated by this project, underlining the fact that there are countless networks of people and computers with goals adversarial to the interests of the U.S. The problem for intelligence analysts is that these networks often reveal themselves only through a coalescence of parts, often temporally and geographically dispersed.

This project posits that network characterization requires methods for identifying hidden properties/relationships and for analyzing network structure; for example, it has revealed that the dynamics of relevant social networks are more important than their intrinsic parameters. Analysts need to be able to predict the evolution of a network's properties. To ensure usability, algorithms are assembled into carefully tested prototypes; three have been developed over the project's course. A human factors team has worked closely with actual



Data plot indicating that an increase in the entropy of certain blogs can be a factor preceding increases in online conversations about violence.

intelligence analysts eliciting their responses to toolkits-in-development, ensuring that refinements reflect real-world applicability. The project has been able to represent and visualize in graphs the uncertainty in network analysis, such as in the small percentage of blogs that can act as "early warning sensors."

### MEGATUX: An Internet Emulation System to Enable Predictive Simulation of Nation-scale Internet Behavior

#### **Ronald Minnich**

The open network structure of the internet can leave critical computers — particularly those of U. S. Government agencies — open to attack by malware such as botnets. These bits of malicious software infect computers on a network, subsequently allowing the originator of the bot to gain control of a nexus of personal computers for a variety of malicious purposes from email spamming to identity theft.

While forensics to detect such malicious activity has been successful in prosecuting some perpetrators, there may be more-efficient ways to detect and thwart or mitigate such activity to reduce its impact. This project is constructing an emulation platform that will allow modeling, analysis, and prediction of the behavior of nation-scale networks of one to ten million machines, which will be self-organizing, as is the Internet. This system will allow introduction of malware,



Geographic map of the network activity of the Sandbot malware developed for this project.

permitting the modeling of attacks that have succeeded against U. S. Government organizations, thereby devising detection and mitigation strategies. A malware prototype known as "Sandbot" has been developed to facilitate this study.

Computation and Simulation

#### Multiscale Models of Nuclear Waste Reprocessing: From the Mesoscale to the Plant-Scale

#### Rekha Rao

With the increased likelihood that nuclear energy will factor into the equation for energy production with a low-carbon footprint, models of nuclear reprocessing plants are needed to support nuclear materials accountancy, nonproliferation, plant design, and plant scale-up.

This project is developing predictive capabilities targeting the design and monitoring of a next-generation nuclear fuel cycle to enable economical large-scale reprocessing with accurate material balances. In addition to plutonium/uranium extraction and separation models — which are being developed at several process scales, from single solution droplet to the contactor device in which extractions occur — plant "flow sheets" will be created. A novel, scalable network model will thus allow coupling of massively parallel contactor models to simple models for other plant unit operations. This will be key to support nonproliferation



Model of turbulent flow within contactor extraction device.

activities, including material accountancy, plant design, and diversion scenarios. Models will be validated through experiments at Sandia and in collaboration with Oak Ridge National Laboratory.

#### Real-time Individualized **Training Vectors for Experiential Learning**

#### **Elaine Raybourn**

Adaptive self-paced and customized "anytime-anywhere" training in intercultural human interaction is one of the top five priority U.S. Army Future Force warfighter outcomes. Consequently, the military extensively utilizes deployed gamebased training around the world. However, military leaders have questioned the metrics that should be used in assessing effectiveness, as well as inquiring whether training can possibly be tailored to the individual warfighter.

This project has been applying Sandia's automated knowledgecapture techniques in an integrated fashion, in order to assess their utility in quantitatively measuring learner expertise and experiential training, the research indicating that these



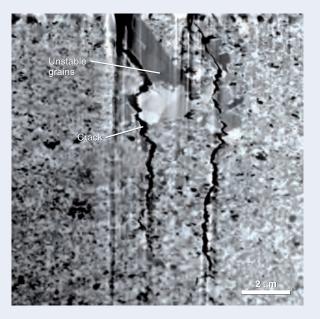
Scenario from one of the evaluated training modules.

techniques can effectively replace human coders of performance. Given the vast amount of training data, such capability would significantly increase data assessment capabilities, and would pave the way for the capabilities of dynamically tailoring training content and feedback to the individual learner.

# Anomalous Suppression of Fatigue and Wear Through Stable Nanodomains Brad Boyce

atigue and wear degradation in engineered metallic structures are pervasive problems, constituting serious drains on the U. S. economy. They are, additionally, concerns for Sandia-designed components in areas as diverse as nuclear weapons components and satellites. Prior work at Sandia has suggested that some nanocrystalline metals can be more resistant to fatigue and wear than conventional alloys, and that perturbing dislocation-length scales is a fruitful approach. For example, research preceding this project suggested that fatigue can possibly be impeded when dislocation-mediated deformation becomes energetically less favorable than other secondary deformation mechanisms. For example, persistent slip bands (PSBs), the atomic-scale precursor to fatigue-crack initiation, may possibly be suppressed by incorporating stable arrangements of dislocation-pinning obstacles at less than the required PSB length-scale.

This project has examined these phenomena—through experiment and modeling—focusing on nanocrystalline alloy composition and dislocation-locking mechanisms that can reduce fatigue and failure and pursuing a path forward to reproducibly engineer improved damage-resistant structures. The project fabricated a nanocrystalline nickel alloy that exhibited a remarkable fatigue life, surviving more than 2.5-million cycles at an enormous peak stress of 1.2 gigapascals. In all nanocrystalline alloys fabricated, crack initiation was preceded by a phenomenon of mechanically induced abnormal grain growth.



Micrograph of cracks initiated in unstable fatiguecoarsened grains in a nanocrystalline nickelmanganese alloy.

The low-friction behavior of nanocrystalline alloys and its concomitant improved wear behavior has been linked to the formation of a tribological bilayer, one component composed of ultrananocrystalline grains (< 5 nm). Modeling was used to explore potential metallurgical scenarios to prevent the abnormal grain growth, and to develop strategies for simulating dislocation-mediated damage processes in granular metals.

# Integrated Optical Phase Locked Loop (IO-PLL) for Attosecond Timing in Microwave Oscillators Anthony Lentine

ompact, low power, and highperformance microwave oscillators are
nearly ubiquitous in microelectronics —
in RADAR, global positioning systems (GPS),
and various other communications devices.
However, their use in systems requiring
high-precision clocking and/or fine phase
resolution tends to be limited by phase noise.
An optoelectronic chip that could improve
this situation by reaching the limits of phase
noise and improve or remove other inherent
noise sources would represent a significant step
forward in this arena.

This project, a close collaboration with the Massachusetts Institute of Technology (MIT), has addressed this issue through a fundamental investigation into the limits of precision timing, with MIT performing benchtop experiments and Sandia focusing on developing an integrated chip-level solution that draws on the capabilities of Sandia's Microsystems and Engineering Sciences Applications facility (MESA) and the Center for Integrated Nanotechnologies (CINT). In developing a process compatible with the Microelectronics Development Laboratory (MDL) that would integrate low-loss silicon waveguides and phase modulators with germanium detectors, the Sandia/MIT team has established a baseline process flow for integration of low-loss waveguides and fiber-to-chip coupling with silicon microphotonic modulators, and has demonstrated a phase noise of -130 dB, 10 Hz from the carrier, leading to 6.8 fs relative timing stability over 10 hours between a pair of 10 GHz microwave oscillators. This represents a new record in relative timing stability, better than any result from the National Institute of Standards and Technology (NIST). The goal

is to ultimately create a chip-scale device to achieve sub-femtosecond timing resolution, an accomplishment that would represent a substantial inroad into that regime of phase-locking.

Michael Watts was the original PI on this project

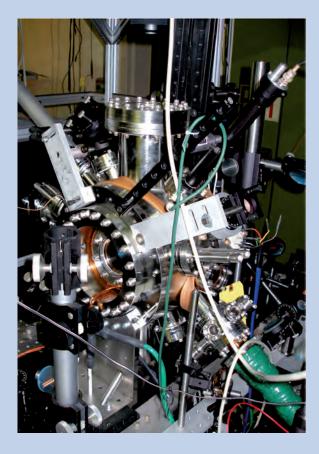
Image of the device engineered in this project.

### Micro-Kelvin Molecule Production

#### **David Chandler**

There are no well-developed techniques for the cooling of molecules from room temperature to microKelvin (less than 1 K) temperature. Such capability would open several areas of scientific discovery including Bose-Einstein condensation of molecules, molecular interferometery, low-energy scattering, and ultrahigh-resolution spectroscopy

This project is pursuing a variation of kinematic cooling to employ a collision to greatly slow the thermal motion of a molecule (0 K representing the absence of thermal motion), much as a cue ball in billiards can come to a complete stop when hitting another ball, by entirely transferring its momentum. By analogy, this project is attempting to collide a molecule with an ultracold (microKelvin) atom of the same mass. There is a finite probability that the collision will result in the transfer of nearly all of the momentum of the molecule to the ultracold atom, thereby lowering the temperature of the molecule near to 0 K. Initial experiments are employing two isotopes of rubidium, <sup>85</sup>Rb, and <sup>87</sup>Rb, as a test case.



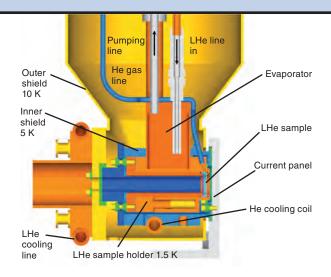
New, higher-flux source for 85Rb constructed to generate larger signals.

# Shock Compression of Liquid He and He-H Mixtures

#### **David Hanson**

Understanding the properties of dense helium has been problematic at very high pressures because of the difficulty of condensing liquid helium samples at very low temperatures on devices such as gas guns, magnetic compression devices, and lasers. This experimental need addresses fundamental physics issues and is also a key to understanding the structure, properties, origin, and evolution of giant planetary interiors.

To solve this experimental dilemma, this project designed and engineered a cryogenic system to condense superfluid liquid helium samples in an appropriate geometry for high-precision equation-of-state (EOS) measurements on the Z accelerator, which possesses the capability to generate the ultrahigh pressures required. The device, based on an evaporation refrigerator, should be expendable, and therefore of reasonable



Schematic of the cryogenic system designed in this project.

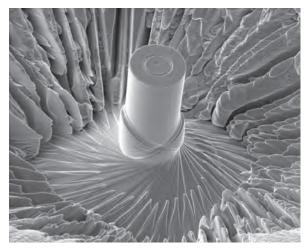
cost and complexity, as well as continuously operating and self-regulating. With these features and requirements accomplished, a new cryogenic capacity on Z will enable very accurate EOS measurements on materials relevant to the weapons program and enhance the experimental capabilities available to theoretical physicists and astrophysicists.

#### An Ion Beam Platform for Screening Materials for Nuclear Reactors

#### **Khalid Hattar**

Reviving fast neutron reactor technology is a key element in creating a viable nuclear energy future. Producing materials tolerant to extensive high-energy irradiation is a requirement for any advanced reactor, but there are no currently operative fast neutron reactors in the U.S.

To address this issue, this project is employing high-energy (MeV) ion irradiation combined with a suite of novel, microscale techniques to characterize the thermomechanical behavior of advanced cladding materials as a function of composition, stress, temperature, and irradiation damage level. For example, the project has developed micropillar compression capabilities for micrometer-sized irradiated volumes. Various other types of experimental-based simulations are also being performed.



Electron micrograph of a self ion irradiated Cu micropillar produced by focused ion beam milling B.L. Boyce).

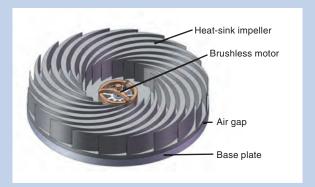
Ultimately, the aim is to clarify the fundamental science behind irradiation damage and mechanical behavior in metallic alloys that will be vital to nuclear fuels modeling efforts and to provide a rapid screening capability for identifying promising new alloys for this extreme environment.

# A Fundamentally New Approach to Air Cooled Heat Exchangers

#### **Jeffrey Koplow**

Air-cooled heat-exchanger technology has remained virtually unchanged for several decades and its inefficiency, noisiness, and propensity to become fouled through dust accretion are limiting factors in technologies such as computer central processing unit (CPU) coolers and environmental cooling systems. In the latter case, such coolers represent an energy inefficiency that is critical, considering today's concern about energy availability and climate change.

This project has designed a novel high-efficiency heat exchanger that is intrinsically immune to fouling by dust because of its high velocity of rotation. The device is based on an air-bearing upon which an impeller rotates. Heat is transferred across a narrow air gap from a stationary heat spreader to the rotating structure, a hybrid of a finned heat sink and an impeller. This places the heat sink boundary layer in a several-thousand-rpm accelerating frame of reference, reducing the thickness of the boundary



layer and providing greatly enhanced heat transfer. The device's "direct drive" generates relative motion between the finned heat sink and surrounding air. This provides a drastic improvement in efficiency and reduces fan noise.

### RapTOR: Rapid Threat Organism Recognition

#### **Todd Lane**

Amid concern about bioterrorism threats to national security from known biothreat agents, there is another imperative to detect unknown biological threats, that is, pathogenic microorganisms not previously encountered and possibly genetically engineered to avoid detection. The technique of ultrahigh-throughput DNA sequencing (UHTS) is capable of characterizing such unknown organisms at the genetic (DNA sequence) level, but only if a suitable sample of the pathogenic organism's DNA is available. This is usually problematic because the nucleic acid (DNA or RNA) of the pathogen exists against a background of the far greater quantity of the infected individual's DNA.

The RapTOR project is designing an automated microfluidics platform that will selectively suppress and subtract the far more numerous human DNA sequences, while amplifying

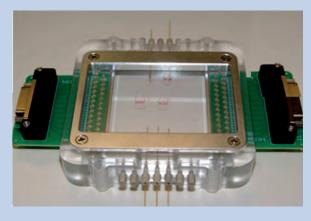


Photo of prototype device.

pathogen sequences. "Normalization" is a hybridization-based process resulting in the preferential destruction of numerically abundant sequences thus increasing the relative abundance of rare sequences. It employs hydroxyapatite capillary-based chromatography, thereby increasing the ratio of pathogen sequences to host sequences such that UHTS can accomplish identification of a threat organism.

#### Reimagining Liquid Transportation Fuels: Sunshine to Petrol

James E. Miller

Domestically produced carbon-neutral transportation fuel: meeting this challenge would be a huge advance toward mitigating global climate change and ensuring energy availability. A direct solution is to recycle the carbon dioxide that results from burning gas, oil, and other fossil fuels by converting it back into hydrocarbons like ethanol, gasoline, and diesel. This is thermodynamically costly, requiring an uphill "push" from some other source of energy.

In this project, solar thermal energy is being applied to supply that uphill push. Concentrated sunlight provides thermal energy to heat redox active metal oxides to high temperatures where they give up oxygen. The resulting reduced metal oxide is then capable of converting chemically stable and unreactive carbon dioxide (CO<sub>2</sub>) to carbon monoxide (CO). This step regenerates the starting oxide and provides the CO for fuel-producing syngas chemistry. Monoliths of the active metal oxides have been developed for the unique

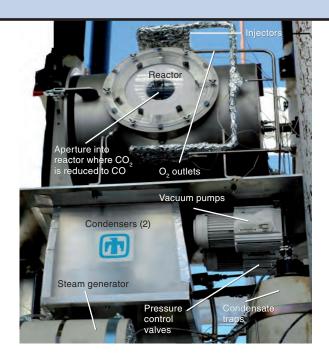


Photo of the CR5 reactor and ancillary structures designed and engineered in this project.

CR5 reactor in which the reaction occurs, a device designed and fabricated as part of this project.

Materials Science & Microsystem Engineering

# SANDIA NATIONAL LABORATORIES

#### **Surface Rheology and Interface Stability**

#### **Lisa Mondy**

Foams have a broad variety of applications connected to Sandia's national security missions, including weapons, explosion suppression, and encapsulation of electronics. Production of suitable foams requires a fundamental understanding of interfacial rheology (flow properties), particularly at the microscale level.







This project studied flow and stability in viscous liquids, with particular emphasis on foams, developing it own Surface Dilatational Rheometer and modeling capability, while also employing commercial instrumentation, in order to develop a comprehensive ability to predict properties of foams and other visco-elastic fluids. One conclusion of the study is that several complementary measurements using different instruments are often required to adequately characterize surfactant systems. This project has resulted in the genesis of an interfacial rheology laboratory at Sandia, including characterization tools with a wide range of sensitivity in surface forces. Such improved understanding of interfacial stability will allow better foams to be produced for a wide range of applications.







44.9 s

Time defoaming=7.2 s

25.9 s

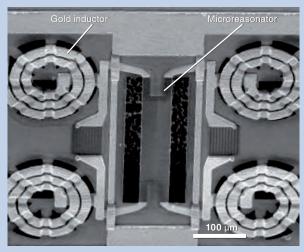
Time sequence of foam generation and subsequent de-foaming.

#### **Featureless Tagging Tacking and Locating:** Micromechanical Resonators

#### **Richard Ormesher**

X-band device applications include various civilian and military tracking and imaging radars in addition to weather monitoring. However, an important subset of such tagging tracking and locating (TTL) devices is limited by the lack of analog signal processing elements at X-band, therefore constraining size and power consumption. This project is developing a low-loss, miniature analog signal processing element at X-band, enabling significant reductions in TTL device size and power.

This project's overall goal is to improve the ability to tag and track adversaries over a broad geographical area, with precision, and with a tag that is physically and electronically very difficult to detect ("featureless"). This portion of the overall project focused on technical advances in microelectromechnical systems (MEMS) acoustic microresonator delay elements. It has developed a novel architecture based on a microresonator with



Micrograph of microresonator with matching inductors developed in this project.

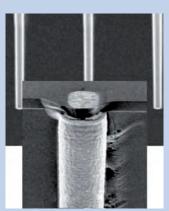
integrated inductors that reduces insertion loss and increases achievable bandwidth.

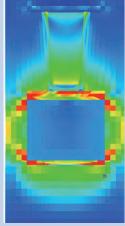
#### 3D Integration Technology for Highly Secure, Mixed Signal, Reconfigurable Systems

#### **Subhash Shinde**

Design of novel system solutions for nuclear weapons components must meet numerous requirements deriving from factors such as harsh environments, smaller component volumes with reduced power budgets, and increased security. These constraints demand novel architecture solutions compatible with existing fabrication technologies that are also reconfigurable as novel surety solutions emerge. Three-dimensional integration of electronic elements is a desirable solution, enabling combinations of separate analog, digital, and other technology functions in a single low-volume package, which can also significantly improve system security.

Utilizing high-fidelity modeling to guide design and processing requirements, this project has devised a low-temperature three-dimensional wafer and chip-stacking capability to provide 3D integrated solutions. In addition to reducing volume and power requirements for electronic subsystems, this approach leverages





Left: Electron micrographs of front-end-of-line through-Si-Vias (FEOL-TSVs) created at Sandia's Microfabrication facility. Right: High-fidelity modeling of fabricationinduced von Mises stress distribution in a vertical and horizontal interconnect (2 million mesh) elements).

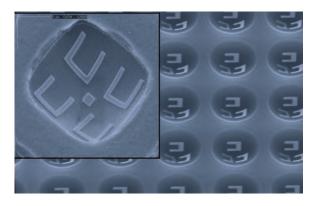
optimized independently developed application specific integrated circuitry while reducing pin count. It also enables multiply redundant subsystems, thus facilitating an adaptive design for meeting security and reliability requirements. Success with bonding dissimilar materials at low temperatures will also benefit other national security applications.

#### **Metamaterial Science and Technology**

#### **Michael Sinclair**

Artificially structured materials not found in nature, metamaterials represent a new frontier in materials science —materials designed and created, through micro- and nanofabrication, with particular performance purposes in mind. Combining modeling, experimentation and fabrication, this project is placing particular emphasis on materials that are nanostructured to respond to specific electromagnetic (EM) frequencies, providing the ability to manipulate the flow of EM energy in ways not achievable with naturally occurring materials.

The project is specifically seeking to manipulate longwavelength infrared (LWIR) in a low-loss fashion. Although metal metamaterials have been constructed with resonances to radio waves and microwaves, designers and engineers have been unsuccessful in the higher-frequency infrared and visible regions of the EM spectrum because metals show high losses

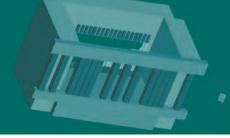


Colorized scanning electron micrographs of newly fabricated three-dimensional metamaterials in the so-called split-ring resonator configuration.

at these frequencies. A novel nanofabrication technique has been developed, known as "membrane projection lithography," one capable of producing 3-D resonator metamaterials with dimensions 100-times smaller than prior fabrication methods.

#### **Coded Aperture Neutron Imaging**

Peter Marleau

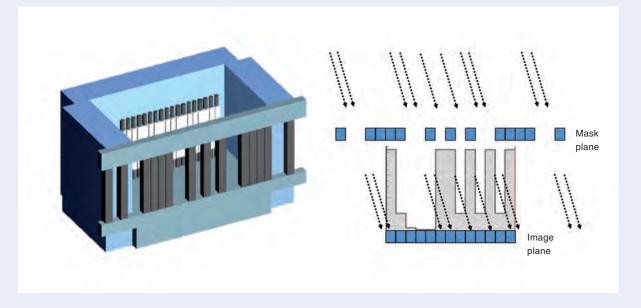


he ability to detect special nuclear material (SNM) over large distances is an important component of homeland security, conferring the ability for early detection of potential nuclear terrorism, as well as aiding verification initiatives. The only reliable means for performing such long-distance detection is through the imaging of the fast neutrons emitted by SNM, neutrons that are energetic enough to penetrate shielding and to travel over long distances without scattering—and whose environmental background is very low.

Previous methods have relied on imaging low-energy neutrons with passive coded apertures, but they cannot adequately modulate fast neutrons. Meanwhile, double-scatter imaging, used to detect fast neutrons has limited detection efficiency. Hence this project combines both double-scatter and coded-aperture methods, that is, active coded-aperture imaging. The mask must be active to increase the opacity to energetic neutrons. One design consists of a mask plane and a position-sensitive detection plane. A source

of fast neutrons within the field of view projects a unique pattern through the mask onto the image detection plane, allowing for the calculation of the source position. The second design consists of a single central detector surrounded by a rotating coded mask, which results in a better signal-to-noise ratio and efficiency of detection.

A set of Monte Carlo simulation tools has also been developed so that experimental results can be assessed against simulations. To illustrate the homeland security potential of the technology, the project team constructed a passive Coded Aperture Neutron Imaging System (CANIS) for use in a large stand-off aircraft screening scenario demonstration. Placed in a 40 ft. sea-land container with a <sup>252</sup>Cf neutron source (IAEA significant quantity of weapons-grade plutonium equivalent) positioned 60 meters away, the detector achieved a 1 in 1000 false positive rate with 90% efficiency in only 15 minutes of dwell time, easily outperforming any technology currently in use. ■



Basic design of the active coded aperture imager.

#### Metabonomics for Detection of Nuclear Materials Processing

#### **Kathleen Alam**

Tracking nuclear materials production and processing, particularly covert operations, is a key national security concern, given that nuclear materials processing can be a signature of nuclear weapons activities by US adversaries. Covert trafficking can also result in homeland security threats, most notably allowing terrorists to assemble devices such as dirty bombs.

Existing methods depend on isotope analysis and do not necessarily detect chronic low-level exposure. In this project, indigenous organisms such as plants, small mammals, and bacteria are utilized as living sensors for the presence of chemicals used in nuclear materials processing. Such "metabolic fingerprinting" (or "metabonomics") employs nuclear magnetic resonance (NMR) spectroscopy to assess alterations in organismal metabolism provoked by the environmental presence of nuclear materials

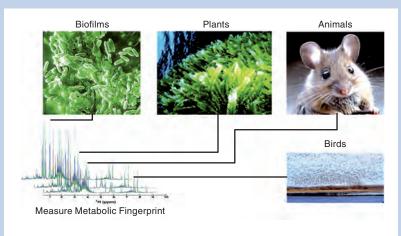


Illustration of the integrated approach that begins with measuring a metabolic fingerprint from a variety of indigenous organisms to allow identification of metabolites serving as signatures of exposure to chemicals involved in nuclear materials processing.

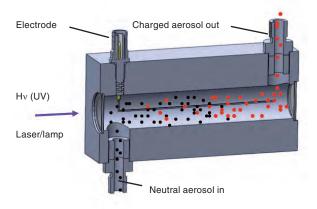
processing, for example the tributyl phosphate employed in the processing of spent reactor fuel rods to extract and purify uranium and plutonium for weaponization.

#### Novel Instrumentation for Selective Photo-Ionization and Trapping of Fine Particles

#### **Ray Bambha**

Very small aerosol particulates are difficult to trap and detect, particularly against the atmospheric background. Examples of important particles include toxic soot aerosols from diesel combustion (typically in the 150 nm size range), trace quantities of uranium in aerosols (potentially indicative of proliferation activities), and biological aerosols possibly connected to bioterrorism

In order to utilize various techniques (e.g., laser-induced breakdown spectroscopy, mass spectrometry) to diagnose the composition and potential significance of such aerosols, these very fine particulates must first be segregated from background. This project has devised a method for such



Drawings of basic design for a device that uses ultraviolet (UV) light to ionize intake aerosol particles, such that they can be separated in an electric field for subsequent analysis.

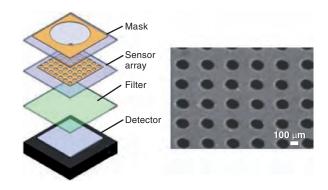
segregation, using ultraviolet (UV) light to photoionize particles, such that the resulting charged particles can then be trapped in an electric field for subsequent analysis. Careful selection of the exact wavelength and intensity of the UV light source has enabled separation of several types of particulate aerosols.

### **Extremely Thin Chemical Sensor Arrays Using Nanohole Arrays**

#### **Igal Brener**

The challenge of designing and fabricating concealable sensors for chemical and biological threats is underscored by the fact that most existing approaches are difficult to miniaturize, requiring either large areas or significant thicknesses. By contrast, this project is developing extremely thin sensor arrays that can be concealed for applications such as space control, surveillance, intelligence, nonproliferation, and armed forces security.

The phenomenon of "extraordinary optical transmission" allows nanohole arrays in thin metallic surfaces to couple incident light to surface plasmons such that a disproportionate amount of light is transmitted through subwavelength-sized arrays. Such transmission is very sensitive to surface chemistry in the vicinity of the holes, meaning that changes in that chemistry can be detected by spectral shifts in transmission. For example, by functionalizing the metal surface with molecules designed to



Drawing of the elements of a nanohole-array sensor (left) and electron micrograph of the array (right).

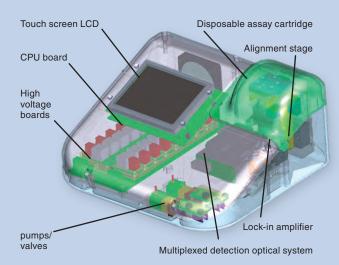
specifically bind chemical explosives, binding of such explosives to the functionalized surface can be readily detected through such spectral shifts with sensors small and thin enough to be easily concealed.

# Deployable Pathogen Diagnostic System

#### **Anson Hatch**

Rapid detection of priority pathogens, either during natural outbreaks or released as an act of bioterrorism is a national security priority, particularly rapid diagnosis at the point-of-incidence to effectively enable a sufficiently rapid response for population protection. Currently, however, diagnosis of affected patients relies on accurate identification of the pathogenic microorganism or its toxins, an often time-consuming process.

This project team has engineered a compact, portable efficient system for pathogen identification, one that relies on membrane-based microfluidic assays interfaced modularly with user-friendly electronics to permit field-based diagnostics by first-responders. A one-square-inch microfluidics chip that snaps into place with electronics interconnects serves as a test



Prototype of the assay platform.

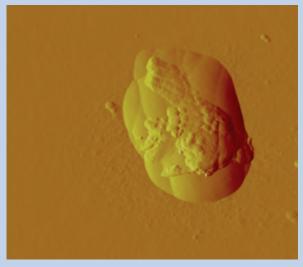
platform. It can be used with any standard immunoassay assay for pathogens or toxins (such as enzyme-linked immunosorbent assay [ELISA]), and it can provide either more-comprehensive touch-screen readouts for biomedical scientists or simpler readouts for first-responders.

### Decontamination of Anthrax Spores in Critical Infrastructure and Critical Assets

#### **Mark Tucker**

Because bacterial spores are extremely difficult to kill by comparison to fully metabolic bacterial cells, current decontamination methods against spores of threat organisms such as *Bacillus anthracis* (anthrax) require the use of highly toxic and/or highly corrosive chemical solutions, such as chlorine dioxide. These corrosive chemicals not only damage materials, but also require complicated, expensive deployment systems.

This project has developed a far less corrosive and less-expensive method for killing bacterial spores in contaminated areas. A novel nontoxic germination solution activates spores, causing them to germinate into vegetative (fully metabolic) bacterial cells. Subsequent to germination, these cells can be far more easily killed than their spores, with relatively nontoxic chemicals such as hydrogen peroxide, alcohols, quaternary ammonium compounds, or other simple treatments such as ultraviolet light.



Micrograph of a germinating spore.

Initial tests have resulted in ~20 million bacterial spores killed on coupons mounted in various locations in a test chamber.

### Field and Charge Penetration by Lightning Burnthrough

#### **Larry Warne**

Many crucial Sandia-engineered electrical systems are threatened by lightning strikes possibly breaching protective metallic enclosures and insulation, thereby interrupting proper function. The design of shielding for safety-critical components depends upon a better understanding of the processes by which such lightning burnthrough occurs, ensuring that critical electrical systems are protected from failure.

This project is seeking to develop a quantitative understanding of the physics that limits voltage and current penetration in lightning burnthrough. One component of this research employs the Sandia lightning simulator, which permits the study of the various phases of electrical discharge associated with a lightning strike. High-speed photography and other detailed instrumentation of these experiments permits diagnostics of the various event phases with submicrosecond resolution. Additionally, the project is developing and applying models for







501.5 ms

### Monitoring lightning effects over microsecond time scales.

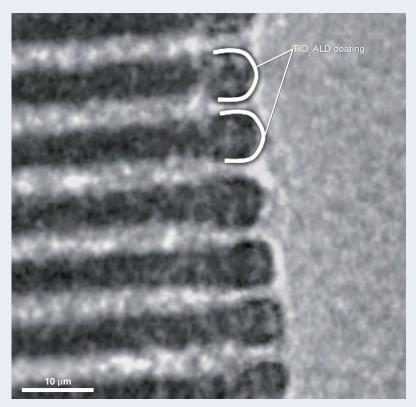
the various physical penetration mechanisms. Ultimately this research will provide a quantitative basis on which to make safety assessments and may permit the development of new methods of protection against lightning strikes.

# Understanding & Optimizing Water Flux & Salt Rejection in Nanoporous Membranes

Susan Rempe

lean water is widely recognized as perhaps the most critical limited resource of this century. Although they have been of great utility in purifying water of salts and contaminants, reverse osmosis (RO) membranes comprise a mature technology, one to which modifications have already shown diminishing returns. New solutions to water purification are required, particularly in the area of efficiency. Pushing water through RO membranes requires energy, and given concerns over global energy shortages, new solutions need to address the fact that purification devices requiring lower energy consumption are crucial.

The lipid bilayers of biological membranes isolate the aqueous compartment inside cells (cytoplasm) from their surrounding aqueous extracellular fluid, the two solutions markedly different in composition. But a controlled flow of water and dissolved ions into and out of cells is mediated through a variety of different protein channels and pumps, each specific to the passage of water (aquaporins) or a given ion. Through study and modeling of biological membranes, this project's researchers have made significant progress in elucidating the chemistry underpinning the specific functionality of these proteins. This project pursued the possibility of modeling and engineering nanoporous inorganic channels to the ion and water selectivity displayed by



Electron micrograph of parallel nanochannels of mesoporous silica, channel entrances precisely tuned by plasma-assisted atomic layer deposition (ALD).

their biological (organic) counterparts. Such nanoporous membranes could be used to purify water completely of its dissolved salts—including those with toxic properties—but might also control the composition of the resulting solution, after passage through the nanoporous membrane, allowing certain salts to remain in the water, thus replicating naturally occurring mineral waters. Modeling has guided experimental work, for example, employing atomic layer deposition (ALD) to chemically modify parallel silica nanotubes as potential water channels.

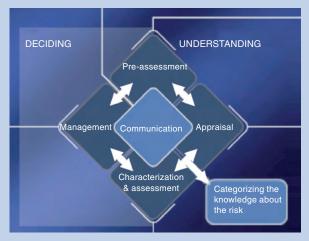
Approaches For A Unified Laboratory Management Biorisk Framework: Responding to Biological Threats Raised by

the Study, World at Risk

#### **Jennifer Gaudioso**

As delineated by the committee on Weapons of Mass Destruction in its published study, *World at Risk*, biological weapons of mass destruction (WMD) pose a grave national security threat, with, for example, terrorists more likely to be able to obtain and use a biological WMD than a nuclear WMD. The study specifically called for bioscience laboratories that handle dangerous pathogens to implement a unified laboratory biorisk management framework. Unfortunately, it has been somewhat difficult to adequately raise awareness in the biological sciences research community of the need for a culture of security regarding the possibility of bioterrorism initiating within that community, itself.

In response, this project is analyzing the value of implementing formal biorisk management within the bio-research community. In addition to studying numerous biorisk cases, the project has addressed issues



The main phases of a laboratory risk-management framework.

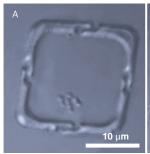
involving management, training, and personnel reliability, in order to measure the effectiveness of risk-management systems, thereby providing a set of precepts as a guide for biorisk management decision-making.

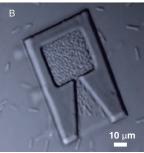
# Development and Characterization of 3D, Nano-Confined Multicellular Constructs for Advanced Biohybrid Devices

#### Bryan Kaehr

Over the course of evolution, Nature has perfected the design of a significant number of biological nanodevices, from sensors to molecular motors to catalysts, photovoltaics and other energy-transformative nanomachines. In certain instances, current initiatives in nanotechnology could benefit from biological solutions. Although most biological devices are constructed entirely or partially of proteins, it should be possible to replicate such structures either completely or partially using inorganic constituents, while retaining functionality for such biohybrid devices.

In this project, mask-directed multiphoton lithography has been used to template biological protein synthesis into specific three-dimensional nanostructures (such as microcantilevers), which have then, in turn, been utilized as structural templates for the multistep conversion to silicon replicas, thereby forming silicon microstructures whose conformation is initially biologically directed. In addition, the mask-directed





Micrographs: A. In situ fabricated protein microenclosure with chicane ports, inside which approximately seven Staphylococcos aureus (round cells) are trapped for a quorum sensing experiment. B. Microchamber filled with a colony of replicating rodshaped (bacilli) bacteria, allowing mechanical analysis of pressure exerted by the colony.

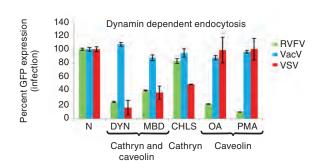
multiphoton lithography technique has been used to construct a diversity of microconfinement chambers for bacterial cells in order to elucidate several key hypotheses about bacterial pathogenicity, cell-to-cell communication, and cell-colony—material interactions.

#### **Genome-wide RNA Interference Analysis** of Viral Encephalitis Pathogenesiss

#### **Oscar Negrete**

Over the past 10 years, the biological phenomenon of RNA interference (RNAi) induced gene silencing has been exploited for biotechnology, therapeutic and basic research science purposes. Most notable is the ability of this phenomenon to determine the specific genes and pathways involved in a biological problem of interest. This project is developing a gene-silencing technology, based on RNAi, in order to investigate the human proteins involved in lethal encephalitis induced by two biothreats — Rift Valley Fever Virus (RVFV) and Nipah Virus (NiV).

By systematically silencing more than 20,000 individual host genes and analyzing their involvement in viral infection, a comprehensive portrait of virus-host interactions should be revealed, that would then allow strategies for therapeutic intervention. The project is developing microfluidic platforms that combine cell and small interfering RNA



Data indicating the probable route of internalization into cells (dynamin-dependent, caveolin-mediated endocytosis) during infection by Rift Valley Fever Virus (RVFV).

arrays for high-level biocontainment compatible RNAi screening adaptable to a molecular-level analysis of other biothreats.

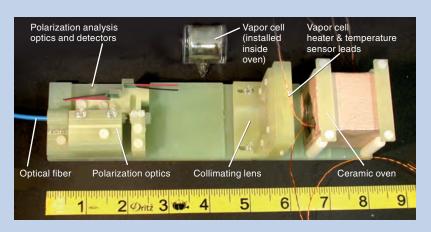
#### **Atomic Magnetometer for Human** Magnetoencephalography

#### **Peter Schwindt**

Current magnetoencephalographic (MEG) imaging of a functioning human brain is difficult because the use of superconducting quantum interference devices (SQUIDS) requires large, cryogenically cooled, expensive hardware. Recently, atomic magnetometers, based on measuring the spin precession of alkali atoms in a magnetic field, have demonstrated

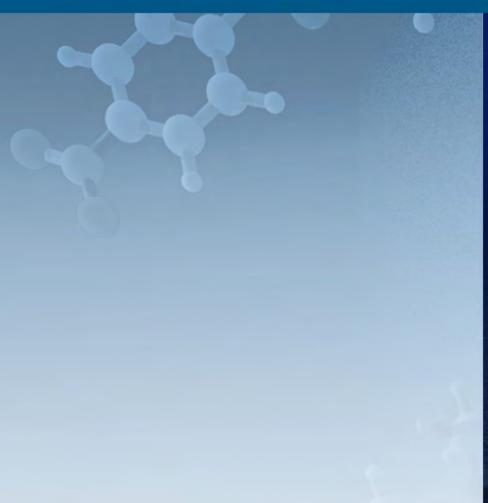
equivalent sensitivity to SQUID-based MEGs. These atomic magnetometers do not require cryogenic cooling, thereby resulting in a much smaller package.

This project, a collaboration with the University of New Mexico and its Mind Research Network, has developed prototype atomic magnetometer for human MEG measurements. The atomic magnetometer reads out the atomic response to a magnetic field through optical interrogation by a laser beam. A single-optical-



axis sensor was developed that utilized a two-color pump/ probe scheme with four-channel output. Its long slender design with a 5 cm x 5 cm footprint on the human head allows high density arraying around the head. The project culminated in the successful measurement of MEG signals with two four-channel sensors on either side of the subject's head. In addition to its primary application in studying human cognition, a portable MEG has potential applications to several other DOE missions.









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